



GREEN'S FUNCTION IN CRITICAL PHENOMENA: DETAILED STUDY OF A STATIC CASE AND A DYNAMIC CASE WITH RESTRICTED GEOMETRY

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ABSTRACT

In Physics, a Green's function $G(\vec{x}, t)$ is a mathematical tool, used to solve differential equations. It is used to relate the response of a system to its cause, and to solve boundary value problems. In the context of critical phenomena, a Green function is a mathematical tool, used to study the response of a system near its critical point T_c to a localized perturbation, which essentially describes how fluctuations in a system propagate through space and time. This provides us crucial information about the behaviour of the system at the critical point, where long-range correlations become dominant. In this communication, we study the use of this function in a critical static case (specific heat) and a critical dynamic case (diffusivity) with restricted geometry separately.

INTRODUCTION

We consider a parallel plate geometry with boundaries at $z = 0$ and $z = L$. Introducing the Fourier transformation through the relation $\psi(\vec{r}, z) = \frac{1}{(2\pi)^2} \int \psi(\vec{k}, z) e^{i\vec{k} \cdot \vec{r}} d^2k$, where \vec{k} is the wave vector in the two dimensional space, the two point correlation function or the Green's function $G(\vec{k}, z, \hat{z})$ is obtained by solving an equation of type

$$\left(\frac{d^2}{dz^2} - k^2 - \kappa^2\right) G(k, z, \hat{z}) = \delta(z - \hat{z}) \quad (1)$$

where $\kappa^2 \propto (T - T_c)$ and T_c , the critical temperature.

The boundary conditions are that the Green's function $G(k, z, \hat{z})$ vanishes at the boundaries and so we can write

$$\begin{aligned} G(k, z, \hat{z}) &= A \sinh az, \text{ for } z < \hat{z} \\ &= B \sinh a(L - z), \text{ for } z > \hat{z} \end{aligned} \quad (2)$$

where $a = (k^2 + \kappa^2)^{1/2}$. Since the Green's function is continuous at $z = \hat{z}$, we have

$$A \sinh a\hat{z} = B \sinh a(L - \hat{z}) \quad (3)$$

and the discontinuity of $\frac{dG}{dz}$ at $z = \hat{z}$ yields

$$-B \cosh a(L - \hat{z}) - A \cosh a\hat{z} = 1 \quad (4)$$

Solving Eqs. (3) and (4), one gets

$$\begin{aligned} A &= -\frac{\sinh a(L - \hat{z})}{a \sinh aL} \\ B &= -\frac{\sinh a\hat{z}}{a \sinh aL} \end{aligned} \quad (5)$$

Using Eq.(5) in Eq.(2), the Green's function are found to be

$$G = -\frac{\sinh az \sinh a(L-\hat{z})}{a \sinh aL} \text{ for } z < \hat{z}$$

$$= -\frac{\sinh a\hat{z} \sinh a(L-z)}{a \sinh aL} \text{ for } z > \hat{z}$$

In a compact notation

$$G = -\frac{\sinh az_{<} \sinh a(L-z_{>})}{2a \sinh aL}$$

If we take a negative sign before the delta function on the right hand side of Eq. (1), i.e.,

$$\left(\frac{d^2}{dz^2} - k^2 - \kappa^2\right) G(k, z, \hat{z}) = -\delta(z - \hat{z}) \quad (6)$$

we get

$$G = \frac{\sinh az_{<} \sinh a(L-z_{>})}{2a \sinh aL} \quad (7)$$

We now use this function in a static case, in particular, the critical specific heat in a restricted geometry.

From thermodynamics, the specific heat at constant volume is

$$C = T \left(\frac{\partial S}{\partial T}\right) = -T \left(\frac{\partial^2 F}{\partial T^2}\right) = T \left(\frac{\partial^2 \ln Z}{\partial T^2}\right) \quad (8)$$

Where $F = -\ln Z$, in the unit of $k_B T = 1$ and Z is the partition function for the system under consideration.

Now, in the Gaussian approximation (which is a model, considers only the fluctuations of the order parameter $\psi(\vec{x})$, but not the interactions between fluctuations of the order parameter $\psi(\vec{x})$), the free energy functional is given by

$$F[\psi(\vec{x})] = \int d^D x \left[\frac{\kappa^2}{2} (\psi(\vec{x}))^2 + \frac{1}{2} (\vec{\nabla} \psi(\vec{x}))^2 - h(\vec{x}) \psi(\vec{x}) \right] \quad (9)$$

where ' D ' is the dimensionality of the space and $h(\vec{x})$ is an external field coupled to the order parameter $\psi(\vec{x})$ linearly.

The partition function is then

$$Z = \sum_{\psi(\vec{x})} e^{-F[\psi(\vec{x})]} \quad (10)$$

Near the critical point T_c , we can substitute the temperature T by T_c and $\delta(\kappa^2) \approx \delta T$ and then Eq. (8) reads as

$$C = C_0 \left[\frac{\partial^2 \ln Z}{\partial (\kappa^2)^2} \right] = C_0 \left[\frac{1}{Z} \left(\frac{\partial^2 Z}{\partial (\kappa^2)^2} \right) - \left(\frac{1}{Z} \frac{\partial Z}{\partial \kappa^2} \right)^2 \right] \quad (11)$$

where C_0 is a constant.

From Eqs. (9) and (11), we get in the limit $h \rightarrow 0$

$$\frac{1}{z} \frac{\partial z}{\partial \kappa^2} = \frac{1}{2} \langle \psi^2(\vec{x}) d^D x \rangle \approx \frac{1}{2} \int \langle \psi^2(\vec{x}) \rangle d^D x \quad (12)$$

and

$$\frac{1}{z} \frac{\partial^2 z}{\partial (\kappa^2)^2} = \frac{1}{4} \langle \iint \psi^2(\vec{x}) \psi^2(\vec{y}) d^D x d^D y \rangle \approx \frac{1}{4} \iint \langle \psi^2(\vec{x}) \psi^2(\vec{y}) \rangle d^D x d^D y \quad (13)$$

Using Eqs. (12) and (13) in Eq.(11), we get

$$C = \frac{1}{4} C_0 [\iint \langle \psi^2(\vec{x}) \psi^2(\vec{y}) \rangle d^D x d^D y - (\langle \psi^2(\vec{x}) \rangle d^D x)^2] \quad (14)$$

We note that the last term on the right hand side of the above equation does not contribute, because they give rise to disconnected Feynmann diagrams. Since the disconnected diagrams of one order get cancelled from the next higher order diagrams, we consider only connected diagrams. Hence we write

$$C \sim [\iint \langle \psi^2(\vec{x}) \psi^2(\vec{y}) \rangle d^D x d^D y] \quad (15)$$

We now approximate the connected correlations (i.e. \vec{x} and \vec{y} are connected) as

$$\langle \psi^2(\vec{x}) \psi^2(\vec{y}) \rangle \approx \langle \psi(\vec{x}) \psi(\vec{y}) \rangle^2 = [G(\vec{x}, \vec{y})]^2 = [G(\vec{x} - \vec{y})]^2 \quad (\text{for translational invariance})$$

Also we introduce two new co-ordinates as

$$\vec{r} = \vec{x} - \vec{y} \text{ and } \vec{R} = \frac{1}{2}(\vec{x} + \vec{y}). \text{ Clearly the transformation Jacobian is } J = -1, \text{ which implies that } |J| = 1 \text{ and so } d^D x d^D y = d^D r d^D R.$$

With all the above discussion in mind, Eq.(15) becomes

$$C \sim \iint [G(\vec{r})]^2 d^D r d^D R = V \int [G(\vec{r})]^2 d^D r \quad (16)$$

Where V is the volume of the D-dimensional space.

It is, however, convenient to work in the k-space. Remembering that the system is restricted in the z-direction with $z = 0$ and $z = L$, Eq.(16) finally takes the form

$$C \sim \int \frac{d^{D-1} k}{(2\pi)^{D-1}} G(k, z, \hat{z}) G(-k, z, \hat{z}) dz d\hat{z} \quad (17)$$

Using Eq.(7) in (17), we get

$$C \sim \frac{1}{a^2 \sinh^2 aL} \int \frac{d^{D-1} k}{(2\pi)^{D-1}} \int dz d\hat{z} \sinh^2 a z_{<} \sinh^2 a(L - z_{>}) = \frac{1}{a^2 \sinh^2 aL} \int \frac{d^{D-1} k}{(2\pi)^{D-1}} I \quad (18)$$

where

$$\begin{aligned}
 I &= \int \int dz dz' \sinh^2 az_{<} \sinh^2 a(L - z_{>}) \\
 &= \int_0^L dz \left[\int_0^z + \int_z^L \right] dz' \sinh^2 az_{<} \sinh^2 a(L - z_{>}) \\
 &= \int_0^L dz \left[\frac{1}{2a} \sinh^2 az \sinh 2a(L - z) - (L - z) \sinh^2 az \right] \\
 &= -\frac{1}{2a} \sinh^2 aL + \frac{L}{8a} \sinh 2aL + \frac{L^2}{4}
 \end{aligned} \tag{19}$$

Using Eq.(19) in (18), the static specific heat for parallel geometry is given by

$$C \sim \frac{1}{L} \int \frac{d^{D-1}k}{(2\pi)^{D-1}} \left[\frac{L}{4a^3} \coth aL - \frac{1}{2a^4} + \frac{L^2}{4a^2} \operatorname{cosech}^2 aL \right] \tag{20}$$

We now study a dynamic case, in particular, the critical diffusivity in restricted geometry. As earlier, we consider a geometry, which is restricted in the z -direction between 0 and L . The surface, perpendicular to the z -direction, is $(D - 1)$ dimensional. Then corresponding to the current density $\vec{j}(\vec{r}, z, t)$, Kubo's formula yields the diffusivity in $D = 3$ as

$$\begin{aligned}
 \lambda &= \frac{1}{L^3 T} \int d^3 r d^3 x dt d\hat{t} \langle \vec{j}(\vec{x}, t) \cdot \vec{j}(\vec{x} + \vec{r}, t + \hat{t}) \rangle \\
 &= \frac{1}{L^3 T} \int d^2 r d^2 x dz_1 dz_2 dt d\hat{t} \langle \vec{j}(\vec{x}, z_1, t) \cdot \vec{j}(\vec{x} + \vec{r}, z_2, t + \hat{t}) \rangle
 \end{aligned} \tag{21}$$

If we consider a liquid-gas system, the order parameter ψ is the density difference between the liquid and gaseous phase and the relevant current density is

$$\vec{j} = \psi \vec{v} \tag{22}$$

where \vec{v} is the velocity field. It should be noted that for the liquid-gas system, the current is proportional to the entropy current and Kubo's formula yields the thermal diffusivity, while for a binary fluid, the current is the mass current and Kubo's formula yields the mass diffusivity [1]. Using Eq.(22) in (21), the thermal diffusivity looks like

$$\lambda = \frac{1}{L^3 T} \int d^2 r d^2 x dz_1 dz_2 dt d\hat{t} \langle \psi(\vec{x}, z_1, t) \vec{v}(\vec{x}, z_1, t) \cdot \psi(\vec{x} + \vec{r}, z_2, t + \hat{t}) \vec{v}(\vec{x} + \vec{r}, z_2, t + \hat{t}) \rangle \tag{23}$$

We use decoupled mode approximation [2] in the above equation and then it becomes

$$\begin{aligned}
 \lambda &= \frac{1}{L^3 T} \int d^2 r d^2 x dz_1 dz_2 dt d\hat{t} \langle \psi(\vec{x}, z_1, t) \psi(\vec{x} + \vec{r}, z_2, t + \hat{t}) \rangle \times \langle \vec{v}(\vec{x}, z_1, t) \cdot \vec{v}(\vec{x} + \vec{r}, z_2, t + \hat{t}) \rangle \\
 &= \frac{1}{L} \int d^2 r dz_1 dz_2 d\hat{t} C_{\psi\psi}(\vec{r}, z_1, z_2, \hat{t}) C_{vv}(\vec{r}, z_1, z_2, \hat{t})
 \end{aligned} \tag{24}$$

As stated earlier, it is convenient to work in the k space, in which Eq.(24) becomes

$$\lambda = \frac{1}{L} \int d^2 k dz_1 dz_2 d\omega C_{\psi\psi}(\vec{k}, z_1, z_2, \omega) C_{vv}(-\vec{k}, z_1, z_2, \omega) \tag{25}$$

The velocity field relaxes much faster and hence in the time scale \hat{t} , the density field changes hardly, so that $C_{\psi\psi}(\vec{r}, z_1, z_2, \hat{t})$ can be considered to remain at its static value and one needs the zero frequency limit of the velocity correlation C_{vv} . Therefore, Eq.(25) takes the form

$$\lambda \sim \frac{1}{L} \int d^2 k dz_1 dz_2 C_{\psi\psi}^{static}(\vec{k}, z_1, z_2) C_{vv}(-\vec{k}, z_1, z_2, \omega = 0) \quad (26)$$

The static correlation for the order parameter ψ is obtained from Eq.(7), which, in the limit $L \rightarrow 0$ and for $z_1 > z_2$ (where $z_1 = z$ and $z_2 = \hat{z}$), is approximated as

$$G \sim \frac{z < (L - z) >}{2L} \quad (27)$$

We now evaluate the zero frequency limit of the velocity correlation function C_{vv} . The relaxation dynamics of the \vec{v} - field is governed by

$$\frac{\partial \vec{v}}{\partial t} = -\Gamma_v \left(k^2 - \frac{\partial^2}{\partial z^2} \right) \vec{v}(\vec{k}, z, t) + \vec{N}_v \quad (28)$$

The velocity field is solenoidal and so $\vec{\nabla} \cdot \vec{v} = 0$. This constraint tells us that we should work with a field \vec{A} , such that $\vec{v} = \vec{\nabla} \times \vec{A}$. If C_{AA} is the correlation function for the field \vec{A} , then the velocity correlation function follows from

$$C_{vv} = \left(k^2 + \frac{\partial^2}{\partial z_1 \partial z_2} \right) C_{AA} \quad (29)$$

To find C_{AA} , we need to introduce the equation of motion for ψ -field. We take this to be a Langevin equation, where the potential corresponds to the free energy functional, given by

$$F = \int d^{D-1}r \int_0^L dz \left[\frac{\kappa^2}{2} \sum_{i=1}^n \psi_i^2 + \frac{1}{2} \sum_{i=0}^n (\vec{\nabla} \psi_i)^2 \right] + \frac{c}{\Lambda} \int d^{D-1}r [\psi^2(\vec{r}, z=0) + \psi^2(\vec{r}, z=L)] \quad (30)$$

Since the anomalous dimension index plays an insignificant role in the study of dynamics, we can work with this quadratic expression for F . Here the geometry is restricted in the z -direction between $z = 0$ and $z = L$. The second term on the right hand side of Eq.(30) is a surface contribution. 'c' is a constant and Λ , an extrapolation length. For $\Lambda \rightarrow 0$, ψ^2 must vanish at $z = 0$ and $z = L$ in order to satisfy the Dirichlet boundary conditions. We set $\Lambda = 0$. For non-conserved ψ -field, Langevin equation now reads as

$$\frac{\partial \psi}{\partial t} = -\Gamma \left(k^2 + \kappa^2 - \frac{\partial^2}{\partial z^2} \right) \psi(\vec{k}, z, t) + N(\vec{k}, z, t) \quad (31)$$

where $N(\vec{k}, z, t)$ is the noise, coming from averaging over the short range fluctuations and is characterized by the correlation

$$\langle N(\vec{k}_1, z_1, t_1) N(\vec{k}_2, z_2, t_2) \rangle = 2\Gamma \delta(\vec{k}_1 + \vec{k}_2) \delta(z_1 - z_2) \delta(t_1 - t_2) \quad (32)$$

If the order parameter field ψ is conserved, there will be an additional factor $\left(k^2 - \frac{\partial^2}{\partial z^2} \right)$ multiplying Γ in Eq.(31) [2]. Then the dynamic correlation function is

$$\begin{aligned} C(\vec{k}, z_1, z_2) &= \langle \psi(\vec{k}, z_1, \omega) \psi(-\vec{k}, z_2, -\omega) \rangle \\ &= \frac{1}{\Gamma^2} \int dz' dz'' R_+(z_1, z') R_-(z_2, z'') \times \langle N(z') N(z'') \rangle \\ &= \frac{2}{\Gamma} \int dz' R_+(z_1, z') R_-(z_2, z') \end{aligned} \quad (33)$$

where

$$R_{\pm} = \frac{\sinh a_{+} z_{<} \sinh a_{+} (L - z_{>})}{2a_{+} \sinh a_{+} L} \quad (\text{From Eq. (7)}) \quad (34)$$

with

$$a_{\pm}^2 = \pm \frac{i\omega}{\Gamma} + k^2 + \kappa^2 \quad (35)$$

To evaluate the integral in Eq. (33), we take $z_1 > z_2$. Then setting $\omega = 0$ and $\kappa = 0$, we get

$$\begin{aligned} C_{AA}(\vec{k}, z_1, z_2, \kappa = 0, \omega = 0) \\ = \frac{2}{\Gamma} \times \frac{1}{4} \left[\frac{\sinh k(L - z_1) \sinh k(L - z_2)}{k^2 \sinh^2 kL} \int_0^{z_2} \sinh^2 kz' dz' + \frac{\sinh k(L - z_1) \sinh kz_2}{k^2 \sinh^2 kL} \int_{z_2}^{z_1} \sinh kz' \sinh k(L - z') dz' + \right. \\ \left. \frac{\sinh kz_1 \sinh kz_2}{k^2 \sinh^2 kL} \int_{z_1}^L \sinh^2 k(L - z') dz' \right] \end{aligned} \quad (36)$$

Clearly,

$$\int_0^{z_2} \sinh^2 kz' = \left(\frac{\sinh 2kz_2}{4k} - \frac{z_2}{2} \right) \quad (37)$$

$$\int_{z_2}^{z_1} \sinh kz' \sinh k(L - z') dz' = \frac{1}{2} (z_1 - z_2) \cosh kL + \frac{1}{4k} [\sinh k(L - 2z_1) - \sinh k(L - 2z_2)] \quad (38)$$

$$\int_{z_1}^L \sinh^2 k(L - z') dz' = \frac{\sinh 2k(L - z_1)}{4k} - \frac{L}{2} + \frac{z_1}{2} \quad (39)$$

On substituting,

$$C_{AA}(\vec{k}, z_1, z_2, \kappa = 0, \omega = 0) = \frac{1}{2\Gamma} \left[\begin{aligned} & \frac{\sinh k(L - z_1) \sinh k(L - z_2) \sinh 2kz_2}{4k^3 \sinh^2 kL} - \\ & \frac{z_2 \sinh k(L - z_1) \sinh k(L - z_2)}{2k^2 \sinh^2 kL} - \\ & \frac{L \sinh kz_1 \sinh kz_2}{2k^2 \sinh^2 kL} + \\ & \frac{(z_1 - z_2) \sinh k(L - z_1) \sinh kz_2 \cosh kL}{2k^2 \sinh^2 kL} + \\ & \frac{\sinh k(L - z_1) \sinh kz_2 \sinh k(L - 2z_1)}{4k^3 \sinh^2 kL} - \\ & \frac{\sinh k(L - z_1) \sinh kz_2 \sinh k(L - 2z_2)}{4k^3 \sinh^2 kL} + \\ & \frac{\sinh kz_1 \sinh kz_2 \sinh 2k(L - z_1)}{4k^3 \sinh^2 kL} + \\ & \frac{z_1 \sinh kz_1 \sinh kz_2}{2k^2 \sinh^2 kL} \end{aligned} \right] \quad (40)$$

The velocity correlation function C_{vv} in the limit $L \rightarrow 0$ is found to be

$$C_{vv} = \frac{1}{2\Gamma} \left[\frac{1}{2k^2 L^2} (4z_2 - z_1) \right] \quad (41)$$

Using Eqs.(27) and (41) in (26)

$$\begin{aligned} \lambda \sim \frac{1}{L} \int d^2 k dz_1 dz_2 C_{\psi\psi}^{static}(\vec{k}, z_1, z_2) C_{vv}(-\vec{k}, z_1, z_2, \omega = 0) \\ = \frac{1}{L} \int d^2 k \int_0^L \left[\int_0^{z_1} + \int_{z_1}^L \right] dz_2 \frac{1}{4k^2 L^2} (4z_2 - z_1) \frac{z_2(L - z_1)}{2L} \quad (z_1 > z_2) \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{4\Gamma L^4} \int \frac{d^2 k}{k^2} \int_0^L (L - z_1) dz_1 \int_0^{z_1} z_2 (4z_2 - z_1) dz_2 \text{ [since, } \int_0^L dz_1 \left\{ \int_0^{z_1} + \int_{z_1}^L \right\} dz_2 = 2 \int_0^L dz_1 \int_0^{z_1} dz_2] \\
&= \frac{1}{4\Gamma L^4} \int \frac{d^2 k}{k^2} \int_0^L z_1^3 (L - z_1) dz_1 \\
&= \frac{L}{96\Gamma} \int \frac{d^2 k}{k^2}
\end{aligned} \tag{42}$$

Thus, for $L \rightarrow 0$

$$\lambda \propto L \int_{\kappa}^{L^{-1}} \frac{dk}{k} \sim L \ln \frac{1}{\kappa L} \tag{43}$$

This result is a bit of a surprise in the presence of a logarithmic term, which can be probed in further study.

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